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Computer Oriented Research

in the

Space Related Sciences

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I. Summary of the Research Work

The primary aim of this multi-disciplinary research program
is to stimulate and broaden the effective use of modern large-
scale, high-speed computers in the University's space research
efforts and to investigate new methods of computer applications
in these fields. In line with this, the program concerns two --
somewhat overlapping -- areas of activity:

1) Research work on the computer oriented phases of a broad
spectrum of space related research projects in close cooperation
with the individual investigators in the different academic
disciplines. Such interdisciplinary research ranges from the
analysis of methods for an effective computational approach
to the problem, to the development of special techniques and
appropriate programs aiding the investigators in all phases
of the project.

2) Research work on basic problems in the computer sciences
to deepen our knowledge and understanding of the most effective
use of computers in research. This includes investigative
work on the development of appropriate programming and monitor-
ing systems and their properties.

During the past half year we have started work on both these
areas of the program. However, it was of course necessary to con-
centrate to some extent on the second problem area, and in parti-
cular on the development of our programming systems, because every
other phase of the project depends crucially upon them.

Following is a summary of our work during the report period.
For more detail we refer in each case to the specific write-up in
Section III of this report.

A. Systems Development

Our efforts in this area centered around the two objectives:
(a) to develop and provide an integrated set of programming
systems under proper monitor control for the most effective
utilization of the entire computer system. This includes the
task of integrating the utilization of the IBM-1401, provided
to us under the grant, into the operational system of our IBM-
7090 installation, (b) to investigate the properties of general
purpose and special purpose algorithmic languages, and to study
associated programming systems and their usefulness in different
research projects.

Our work in the first of these two areas has been very successful and has provided us with a very satisfactory and highly efficient set of programming systems. From the beginning we decided to direct our efforts mainly to those systems which can be operated under complete control of one central monitor. As such a monitor we chose the IBM basic Monitor (IBSYS) and this choice has proved to be a very fortunate one, assisting from the beginning in the proper and effective utilization of the entire computer system by the individual projects of this research program.

Work has also started on the analysis of special languages and associated programming systems. Developmental work is underway to connect several of these systems to our monitor system, in order to make them available and useful to different research projects. Other work concerns the development of special programming packages, in particular for multi-precision work and for the effective utilization of macro-instructions. Two reports are presently being written describing some phases of this work.

B. Computer-Oriented Research

In the report period we began work on the computer-oriented phases of the following research projects:

1. ### Numerical Mathematics

   a) Chebychev approximations for elementary and special functions
   b) Numerical analysis in modular arithmetic computers
   c) Computer applications to group theory
   d) Investigations in logic and number theory using a computer.

2. ### Chemistry

   a) Crystallographic structure determination by computers

3. ### Molecular Physics

   a) Computation of Vibration-Rotation Matrix Elements for diatomic molecules

4. ### Physics and Astronomy

a) Computer program development in long wavelength
    radio-astronomy
    b) Computational methods in nuclear physics

5. Chemical Engineering

    a) Investigation of complex equilibrium stage processes
    b) Computer modeling of two-phase flow problems

As previously mentioned, descriptions of these individual
projects are given in Section III. The work in numerical mathe-
matics and chemistry has already produced significant results
which will be presented in several reports now in various stages
of completion. One phase of the work in nuclear physics is ex-
pected to appear in book form.

Research work on other projects and with other departments
is now beginning. In particular, we are discussing with the
Department of Electrical Engineering cooperative work on two
projects: (a) exploratory research on the problem of semi-auto-
matic indexing and association of documents in depth and in a
carefully defined area. Initially this will involve computer
research on the structure of the particular information space,
and of suitable formal languages for manipulating that space
on a computer; (b) investigative work concerning certain pro-
blems in the area of the number and structure of unit-distance
codes.

The Computer Science Center itself is preparing to enter the
research area of pattern recognition and pictorial data-pro-
cessing. At the same time the Department of Psychology is begin-
ning a research project on human pattern recognition. Our own
plans revolve around the investigation of possible statistically
based generalizations of the edge concept, the definition of
"enhancement" operations for such generalized edges, the testing
of these results by computer simulation, and related problems
that may develop. The Psychology project is concerned with the
fact that the human observer's ability to recognize patterns under
degraded (noisy or poor quality) conditions is not clearly under-
stood. Although many studies have demonstrated the importance
of information content, redundancy, and "meaningfulness" in form
or pattern recognition, further specification of the interactive
effects of these variables in recognition tasks using degraded
visual stimuli is necessary to understand more clearly the pro-
cessing mechanisms involved in human pattern recognition. Ex-
periments in this area depend crucially on the computer because

only the computer can generate sufficiently complex classes of visual stimuli for given specifications as to information content, noise, and quality. These forms will then be judged by subjects for "meaningfulness" using multi-dimensional psychophysical scaling techniques and verbal descriptions (associations). The experimental studies will also include evaluation of the effects of these stimulus variables on human pattern recognition in various perceptual tasks. The analysis of the experiments will of course again involve computer use.

II. Personnel

Dr. W. C. Rheinboldt, Director of the Computer Science Center and Research Professor of Computer Science is the principal investigator of the entire program. The systems development work is handled by Alfred E. Beam, Senior Systems Analyst of the Computer Science Center in cooperation with John P. Menard, Assistant Director of the Computer Science Center. In August 1963, Dr. Earl J. Schweppe joined the Computer Science Center as Research Assistant Professor of Computer Science. His interests are in the study of special algorithmic languages and associated programming systems, and in particular the investigation of man-machine systems. The systems development group also includes George E. Lindamood, who joined the Center as a Research Programmer in September 1963. In July 1963, Dr. Alan Marcovitz of Columbia University joined our Center to cooperate in certain phases of the analysis of the Michigan Algorithmic Decoder. Dr. Marcovitz is now Assistant Professor of Electrical Engineering at the University of Maryland and is continuing his cooperation with the program.

In June 1963, Dr. A. Sinkov, Associate Professor of Mathematics and Research Consultant in the Computer Science Center left the University to go to the Arizona State University. His place has now been taken by Dr. Richard Austing of Catholic University, who joined the Center in September 1963 as Research Assistant Professor of Computer Science. Dr. Austing's special interests are in Numerical Mathematics.

Mr. C. K. Mesztenyi, Senior Research Programmer at the Computer Science Center is continuing his work on rational approximations, and he is also directing the programming work connected with the research program. Under his guidance, R. L. Clark, Research Programmer and A. Radichevich, Jr. Research Programmer, are working on special programming problems, particularly the development of multi-purpose programs for use by different research projects.

The following Graduate Research Assistants have been connected with the program during the Spring Semester 1963: J. Connelly (Mathematics), G. Meyer (Mathematics) and S. Wax (Mathematics). C. Park (Chem. Eng.) and F. Karriker (Physics) worked with us full time during the summer, and beginning with this new academic year we have the following graduate research assistants participating in the activities of the program: J. Connelly, F. Karriker and C. Park. It should be noted here that two of the 20 NASA Trainees

are working in computer-oriented mathematics: J. W. Snively,
Jr. and J. Maryak. Both these students have associated themselves
with research projects under this program and both are presently
writing their masters' theses on certain aspects of these projects.

In line with the multi-disciplinary character of the entire
research program we have the benefit of collaborating with a num-
ber of colleagues in the University of Maryland. Their names are
listed with each of the specific projects in Section III. In addi-
tion, we would like to mention the names of several colleagues who
are cooperating particularly intensively in our efforts under this
program: Dr. T. B. Day (Physics), Dr. J. M. Stewart (Chemistry),
Dr. S. Weissman (Molecular Physics), Dr. N. Anderson (Psychology),
Dr. H. Tompkins (Electrical Engineering), and J. Chappell, Jr.
(Business Data Processing). Finally, we would like to list the
name of Mr. G. Berns, IBM-Technical Representative at the Computer
Science Center whose cooperation with our systems programming group
is a great help in our work.

III. Detailed Descriptions of Supported Projects

A. Programming Systems

A. Beam, J. Menard, Computer Science Center
G. Berns, IBM

The effective utilization of modern complex large-scale computers depends crucially on the availability of versatile programming and monitoring systems. Especially for a multi-disciplinary research program such as ours, the proper selection, adaptation, and diversification of highly flexible programming systems is of extreme importance. Accordingly, we concentrated heavily on the development and modification of such systems.

As mentioned in Section I, our work has been based on the IBM Basic Monitor (IBSYS). A diagram of all the programming systems now available at our Center under the IBSYS Monitor is given at the end of this section, Fig. 1. All these systems have been integrated into a operational package especially suited to the configuration of our equipment and the special needs of our research program. A second diagram, Fig. 2, indicates all the other systems which are operational and available upon request to the researchers using our facilities.

The systems-configurations described in Figures 1 and 2 contain certain special features and modifications which we developed with the particular aim of meeting the extremely varied demands of our research work. A Multiple Precision Package (MPP) -- an extremely useful tool in performing computations where extensive accuracy is needed or where the range of the data is extremely large -- has been incorporated under IBSYS and is available in conjunction with the FORTRAN II Monitor. For ease of operation and to give greater accessibility to the MPP, a language called PRECISE has been developed and is also available under IBSYS. PRECISE has been patterned after and is closely related to the OMNITAB language developed at the National Bureau of Standards. The essential difference is that OMNITAB performs its arithmetic operations in a single precision mode. Both languages have proven very useful to different research projects in the University. We have therefore agreed to cooperate with the authors of OMNITAB in modifying the OMNITAB program and incorporating it under IBSYS. A target date of 1 December 1963 has been set for this project.

Several research projects are now developing which will need symbol-manipulating and information-processing languages. For this reason we have already incorporated the well known IPL-V language into the IBSYS Monitor, and we have now also modified the LISP-System developed at MIT, and incorporated it into the IBSYS Monitor.

A further aspect of the research in the programming systems field has been our detailed study of the capabilities of the basic IBM programming systems. In particular, we have given very special attention to the Macro Assembly Program (IBMAP). The results of this research are embodied in a system called MOIST (Macro Output Input System) which was developed at the Computer Science Center by Mr. G. Berns. As indicated by its name, the purpose of MOIST is to provide an extremely flexible and simple means for programming input and output for the IBM 7090/94. MOIST has been written using IBMAP and operates under the IBJOB Monitor under IBSYS. A second version MOIST-F is in preparation for operation under the FORTRAN Monitor System. A complete report on MOIST will be forthcoming.

With the increasing importance of algorithmic languages we have found it necessary to devote a considerable amount of time to this area. The SHARE organization, together with IBM, has recently released an ALGOL compiler for the IBM 7090. This compiler is presently operating under FORTRAN II, Version 2. Our immediate concern has been to investigate the usefulness and efficiency of the compiler. At the same time we are proceeding with the task of modifying the compiler in order that it may operate under the IBSYS Monitor. No target date has been set for this task.

Further efforts with algorithmic languages have been concerned with the MAD (Michigan Algorithmic Decoder) language. The extreme speed of compilation and the flexibility and power of the language make this a very useful tool for research. We have made this language available to our users under its own separate system (Michigan Executive System) and we are presently modifying the MAD Compiler and writing a special monitor similar to the FORTRAN Monitor System which will allow the MAD Compiler to operate under IBSYS. The target date for completion of this project is 1 February 1964. It is expected that such a modification will find very wide acceptance and serve a very useful purpose.
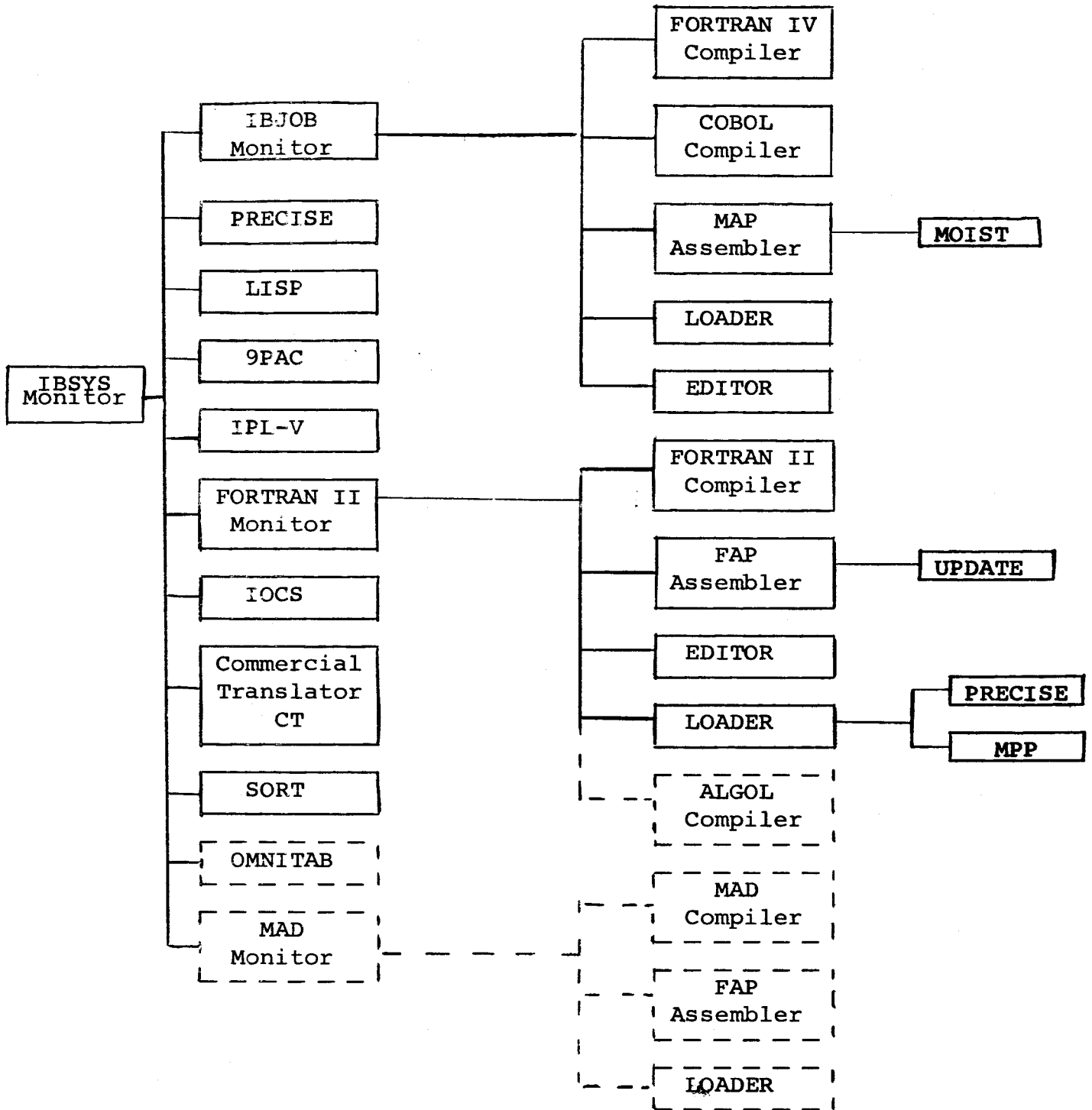
Primary Operating system at the Computer Science Center. Dashed lines indicate those systems presently being made operational under the IBSYS Monitor.

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┌──────────────┐      ┌──────────────┐                              ┌──────────────┐
│ Michigan     │──┬───│     MAD      │        ┌──────────────┐   ┌───│  FORTRAN II  │
│ Executive    │  │   │  Compiler    │        │  FORTRAN II  │   │   │  Compiler    │
│ System       │  │   └──────────────┘        │  Monitor     │───┤   └──────────────┘
│ Monitor      │  │   ┌──────────────┐        │ (Independent)│   │   ┌──────────────┐
└──────────────┘  ├───│   FORTRAN    │        └──────────────┘   ├───│    ALGOL     │
                  │   │(non-standard)│                           │   │  Compiler    │
                  │   │  Compiler    │                           │   └──────────────┘
                  │   └──────────────┘                           │   ┌──────────────┐
                  │   ┌──────────────┐                           ├───│     FAP      │
                  ├───│    UMAP      │                           │   │  Assembler   │
                  │   │  Assembler   │                           │   └──────────────┘
                  │   └──────────────┘                           │   ┌──────────────┐
                  │   ┌──────────────┐                           ├───│    EDITOR    │
                  ├───│    COMIT     │                           │   └──────────────┘
                  │   └──────────────┘                           │   ┌──────────────┐
                  │   ┌──────────────┐                           └───│    LOADER    │
                  ├───│    IPL-V     │                               └──────────────┘
                  │   └──────────────┘
                  │   ┌──────────────┐
                  ├───│   UTILITY    │
                  │   │    FILE      │
                  │   └──────────────┘
                  │   ┌──────────────┐
                  └───│    LOADER    │
                      └──────────────┘

┌──────────────┐      ┌──────────────┐
│    BELL      │──┬───│   FORTRAN    │
│   Monitor    │  │   │(non-standard)│
└──────────────┘  │   │  Compiler    │
                  │   └──────────────┘
                  │   ┌──────────────┐
                  ├───│    BEFAP     │
                  │   │  Assembler   │
                  │   └──────────────┘
                  │   ┌──────────────┐  ┌──────────────┐
                  └───│    LOADER    │──│   OMNITAB    │
                      └──────────────┘  └──────────────┘
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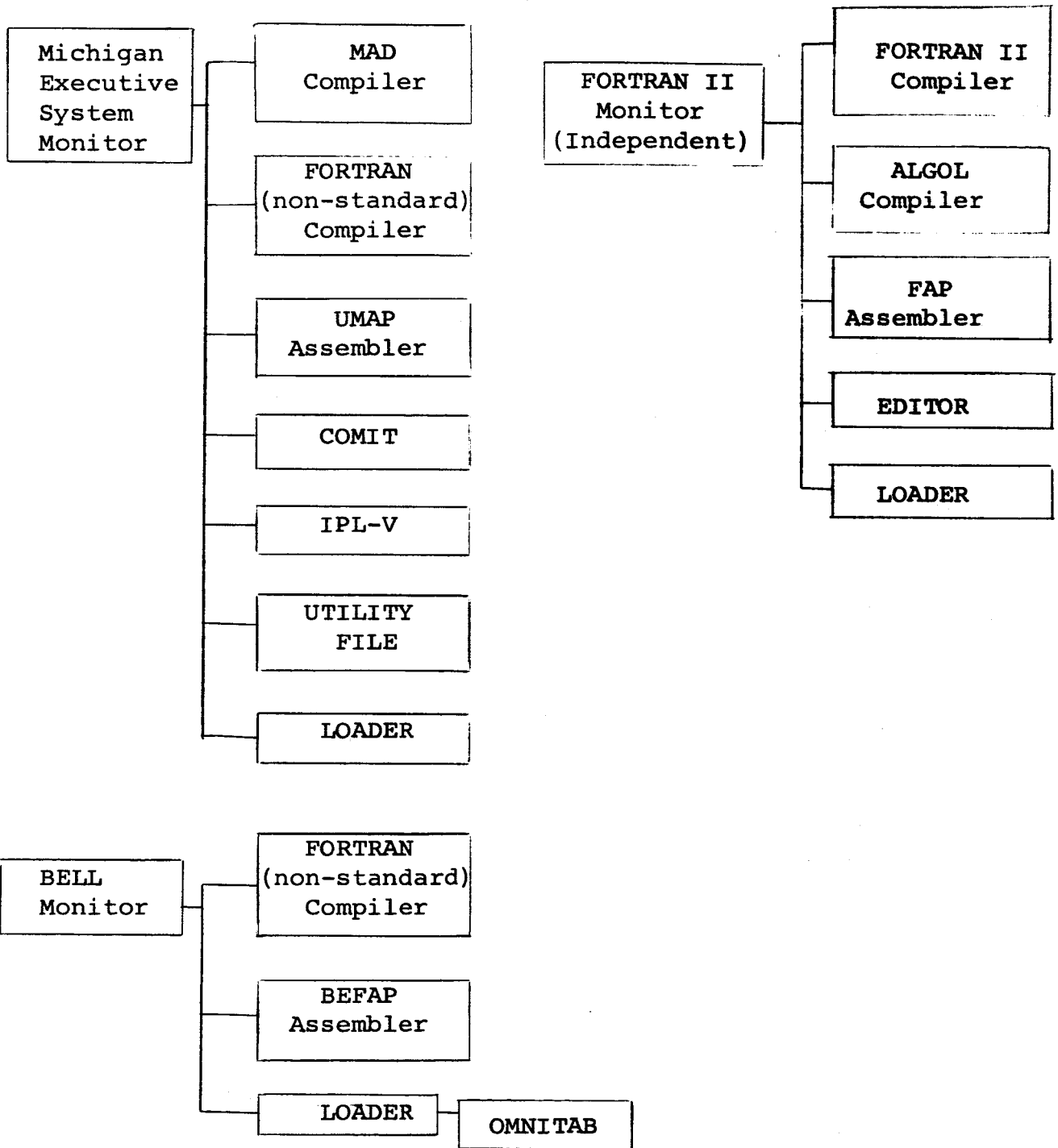
Fig. 2

Other systems that are operational and
presently available upon request at the
Computer Science Center.

B. Computer-Oriented Research Projects

1) Numerical Mathematics

a) Chebyshev Approximations for Elementary and Special Functions

C. K. Mesztenyi, Computer Science Center
Dr. C. Witzgall, National Bureau of Standards

In all computational work elementary and special functions need to be evaluated repeatedly and efficiently. This has led in past years to an extensive development of approximations for these functions. One large-scale research project on the use of rational approximations for the uniform (Chebyshev) approximation of functions was carried out by H. Maehly at Princeton University and later on at Syracuse University. Dr. Maehly's death in 1961 interrupted this work after only a small part of the research results had been completely checked out and published. His direct collaborators, C. Witzgall (now with the Applied Mathematics Division of the National Bureau of Standards) and C. K. Mesztenyi (Senior Research Programmer at the Computer Science Center) are now collecting these earlier results in order to put them in final form for publication and then to continue this important research work.

During the past half year, C. Mesztenyi has been concerned with the numerical check-out of the rational approximations obtained by Maehly and with the experimental investigation of their actual error-curves. Computer programs have been completed for the multi-precision evaluation of these formulas and for their comparison with the exact functions. This work is expected to continue for another four to five months and the results are expected to be published in book form.

The multi-precision part of the computational work involves the use of a special multi-precision programming package developed and perfected by A. E. Beam, Senior Systems Analyst of the Computer Science Center. This multi-precision package will be described in a separate report.

After the work on Maehly's rational approximations has been completed and published, both investigators plan to continue their earlier work on special iterative methods for obtaining approximations of given functions.

b) <u>Numerical Analysis in Modular Arithmetic Computers</u>

G. E. Lindamood, Computer Science Center

Modular arithmetic computers--digital computers in which numbers are represented by their residues with respect to several mutually prime moduli -- have recently been the subject of considerable investigation in several universities and private companies in the United States and in the Laboratory of Mathematical Machines in Prague, Czechoslovakia. Of particular interest in these investigations have been the theoretical problems arising in performing several fundamental operations, such as overflow detection, magnitude comparison, and division, in these computers.

As a result of work beginning in June 1962, at Westinghouse Electric Corporation in Baltimore, Maryland, G. E. Lindamood has found mathematical techniques for comparing the magnitudes of two numbers, detecting additive and multiplicative overflow, performing division, and extracting square roots in modular arithmetic computers. These techniques are of the utmost importance in the development of modular arithmetic computers, since it was previously unknown how to perform these operations in the number system used in such computers. To demonstrate the practical application of these techniques, G. Lindamood prepared programs to simulate modular arithmetic division and square root extraction on the IBM 7090 computer. These programs, which were run on our 7090 computer, have provided additional information about the speeds of convergence and general behavior of the modular arithmetic division and square root techniques.

G. Lindamood has recently joined the staff of the Computer Science Center as a Research Programmer and is currently preparing a report summarizing his contributions on performing fundamental operations in modular arithmetic computers and presenting the results of the simulation runs. The report will serve as the thesis for his M.A. degree in mathematics and will later be published in the form of several articles in professional journals.

<u>Pertinent References</u>

G. Lindamood & G. Shapiro: "Magnitude Comparison and Overflow Detection in Modular Arithmetic Computers" <u>SIAM Review</u>, to appear (in Oct. or Nov. 1963 issue.)

c) Computer Applications to Group Theory

Dr. A. Sinkov, Computer Science Center*
J. W. Snively, Jr., NASA-Trainee, Computer Science Center

In the last few decades, group-theoretic problems have
gained increasing importance in a number of applications,
ranging from quantum-mechanics to cryptography. But only
in recent years has attention been directed toward the use
of computers in group-theoretic research.

A basic problem in the theory of groups is the determin-
ation of the group defined by a set of relations satisfied
by its generators. The coset enumeration technique of Todd
and Coxeter (Proc. Edinburgh Math. Soc. (2), 5, 1936) is
sufficiently mechanical to admit of being programmed for a
high speed computer. Several investigators have worked at
the problem of programming it. Most of this work is as yet
unpublished. A first paper concerning this topic was pub-
lished by J. Felsch, (Num. Math. 3, 250, 1961); he used a
Zuse Z-22 computer. Recently a paper by J. Leech (Proc.
Cambridge Phil. Soc. 59, 257, 1963) described his work on
the EDSAC-computer. During the past half year the investi-
gators developed IBM-7090 programs for this enumeration pro-
cess.

A comparison of these three programs is available for the
case of a test problem; namely, for the enumeration of a
group defined earlier by A. Sinkov (Annals of Math. 38, 3,
1937). A pencil and paper enumeration by Todd required in
excess of 30 hours, Felsch used 2 hours on the Z-22, Leech
used 42 minutes on the EDSAC and Sinkov used 5 minutes on the
IBM-7090.

This enumeration procedure is being used to study the
Burnside problem of exponent 4, about which very little is
known. $B_{4,1}$ is trivial and of order 4; $B_{4,2}$ is of order
2^{12}. The only other known result is that $B_{4,n}$ is finite.

The IBM-7090 programs for the computer enumeration have
produced the following results to date:

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1. An irreducible definition of the 2-generator methabelian group of exponent 4.

2. The order $B_{4,3}^{(3)}$ (where the superscript means that 3 generators are involutary) is 2^{10}.

3. The order of $B_{4,3}^{(2)}$ is 2^{21}.

4. A procedure has been indicated by which the orders of $B_{4,n}^{(2)}$ may be derivable from the establishment of a chain of invariant operators and corresponding quotient groups. These invariant operators -- for all cases tried thus far -- are commutators or squares of commutators.

5. This procedure -- if effected -- will simultaneously provide a definition of a Burnside group of exponent 4 for every power of 2 from that which gives the order of $B_{4,n}^{(x)}$ down to 2n-x.

6. It is indicated that the extension from $B_{4,n}^{(a)}$ to $B_{4,n}^{(a+1)}$ causes the exponent of 2 to be at least doubled.

A preliminary report by A. Sinkov will appear shortly, describing these results in more detail. Another report, currently being written by J. Snively, presents further details about this research work. Although Professor Sinkov has left the University, he is still directing Mr. Snively's thesis work in this topic.

d) Investigations in Logic and Number Theory Using a Computer

Dr. S. Kuroda, Department of Mathematics
John Maryak, NASA-Trainee, Computer Science Center

Although they may seem to belong to different areas of mathematics, Logic, Number Theory, and Computer Science are intrinsically related fields. For example, it is certainly no accident that the idea of applying Boolean algebra to the analysis of switching circuits developed independently in the United States, Russia, and Japan around 1940. Since that time, the three fields have grown closer and closer together.

Recently there have been remarkable advances in algebraic number theory by computational methods (see, e.g., H. Cohn, O. Taussky, Number Theory, Chapter 16 of J. Todd, Survey of Numerical Analysis). Even so, more computational results are needed

to prepare for further theoretical progress in this field. For example, the rational primes of the form

$$q = (p^r - 1)/(p^d - 1) \qquad \text{(p rational prime)}$$

have gained added importance due to their appearance in Waring's problem.

One of the aims of the present investigation is to clarify structures of the ideal class groups of cyclotomic fields. $Q(\mathfrak{Z}_m)$ generated by a primitive mth root of unity $\mathfrak{Z}_m$ where m is a positive integer related to the primes mentioned above. A related problem involves the determination of the decomposition law of rational primes in various algebraic number fields.

The computer-oriented phase of this research involves as a first step the calculation of prime number tables, more extensive than those generated up to now. This in turn leads to interesting computer science problems in bit-manipulation.

During the past half year a set of computer programs has been developed to calculate a table of all prime numbers less than 4.29 billion in a form suitable for further computations. Each bit-position in a buffer area B consisting of M words represents from left to right in ascending order of storage, the odd integers (2N + 1) through (2N • 72M - 1), where N is a given positive integer divisible by 36 (word-length of the IBM 7090). The program uses the Eratosthenes-sieve method to set to 1 all bits representing primes, and to set to 0 all those bits representing composite numbers. All programs have been developed to assure the utmost efficiency, proper generality, and usefulness in further number-theoretic and logical computations. It is particularly noteworthy that the programs are extremely fast. For example, to compute a table of prime numbers in an interval of about 1.8 million numbers takes only between 39 seconds to 140 seconds, depending on the location of the interval in the total range from 0 to 4.2 billion.

A special report describing these programs and the special bit-manipulation techniques is in preparation. Professor Kuroda is now beginning to use these programs for his research work mentioned above. Similar bit-manipulation techniques will be important in a second phase of the entire project concerning the proving of mathematical theorems on a computer.

2. Crystallographic Structure Determination by Computers

Dr. J. M. Stewart, Department of Chemistry and Computer Science Center

The problem of determining the structure of crystals is one of great interest to Chemists, Biologists, and Geologists at the present time. This research project is directly concerned with the development of methods and corresponding computer programs for the accurate determination of the atomic parameters in crystals from X-ray or neutron diffraction data of solid crystalline material. Since the data gathered are the result of diffraction rather than refraction, the use of high-speed computing facilities are of crucial importance to the practicality of the method for investigating the structure of the many interesting compounds.

In the beginning of programming for the solution of crystal structures, it was a common practice to write isolated programs for each application. However, as data gathering techniques improved and became more automated, it became quite obvious that the programming methods would also have to improve and become more automatic. The programs developed here have accomplished this goal and form a much needed crystallographic computing system.

More precisely, the programs are designed to constitute a "system" for X-ray crystallography which will run independently of, or in conjunction with, existing IBM-709 - 7090 - 7094 monitors. The major subroutines of the system do the calculations necessary to interpret X-ray diffraction patterns and to establish accurate atomic parameters in crystals.

The course of the computation, which may involve any number of the links in the system, is controlled by the sequence of cards in the input data. These control functions are exercised by a special subroutine called "CALLER" through which all input passes. Input data cards are identified by punches in the first six card columns, usually a mnemonic of the card function. A data deck consists of the following kinds of cards:

    (a)   Operational cards (which are acceptable at any time) perform immediate operations such as assigning tapes, printing remarks and instructions and supplying a title.

b) A calling card serves to call the specified program link and initiate the program.

c) Data cards to be used under control of the program and to supply, for example, parameters, intensity data, and control information.

d) An end card indicating the end of the data deck.

A sequence of <u>interdependent</u> calculations may be performed by stacking up an appropriate set of data decks (for example, "parameter loading" followed by a "Fourier synthesis," or several cycles of "automatic refinement"). This set of data decks is identified by a preceding special card, the *-data card. Another <u>independent</u> sequence of calculations may be initiated by following the first sequence by another *-data card and one or more data decks - et continuum. Execution terminates and control is returned to the calling monitor when a "FINISH" card or an END-OF-FILE is read on the monitor input tape.

At the present time, the X-ray crystallographic computing system is partly completed and has been distributed for use at the Universities of Maryland, Washington, and Florida, as well as at the Naval Research Laboratory, Washington, D.C., The NASA-Space Center, Huntsville, Alabama, and the National Bureau of Standards, Washington, D.C.

The list of program links at the end of the section serves to illustrate the present and intended scope of this crystallographic computing system for the IBM-709 - 7090 - 7094.

The major responsibility for the "X-ray 63" programming system lies with J. M. Stewart (University of Maryland) and Darrell High (University of California at San Diego). The programming as a whole has been the result of group effort by many people. J. Stewart is currently preparing a report giving a complete description of the system and the methods used.

This list is the table of library programs in the "X-ray 63" programming system. An asterisk refers to the programs currently included in the working system tape.

*	LOADER	Beginning program, tape generation
*	FC	Parameter loader and statistical calculation of structure factors
*	DIFSYN	Differential synthesis
	DFSYNA	Modified differential synthesis
	LSQFM	Full-Matrix least squares
*	ORFLS	Busing-Martin-Levy full-matrix least squares
*	FOURR	Fourier synthesis
*	FOUREF	Fourier refinement (shifts atoms to Fourier peak)
*	SHLPAT	Shell Patterson
	BONDLA	Bond length and angles
	PROJCT	Projection of a molecule on a plane
*	LSQPL	Least squares, plane and line.
	SUPTAP	Preparation of superposition binary tape
	SUPERA/SUPERB/SUPERC	Patterson superposition programs A, B and C
	SUPROT	Rotation program to fit model to Patterson
*	DELSIG	Plot of delta-F versus F-observed for sigma for data reduction
	PHASE	Calculation of Karle-Hauptman phases
*	DATRDN	Data reduction
	DATCOR	Data correlation for films
*	DATFIX	Calculation of scaled unitary structure factors
*	MODIFY	Search and modify reflection tape
	WEIGHT	Prepare weights for least squares
*	ESORT	Sort for Karle-Hauptman phase determination
	LISTFC	Final structure factor listing
*	CRYSET	Donnay-Takeda crystal transformations
*	RPLANE	Calculate R over a projection for moved molecule
	RLIST	Calculate R for special classes of reflection
	PARAM	Least-squares refinement of lattice parameters
	TFINFO	Calculates temperature factor statistics
	GESET	Generation of reflection and crystal set for GE XRD-5
	REFPAK	Interconverts reflection tape and binary deck
	REFSOR	Reflection sorting from tape
	TAPCOP	General tape copying routine
	PATCON	Patterson convolution program
*	BYEBYE	Convert system reflection tape to non-system formats
	NRLA/NRLB	Spare entry A or B, respectively for experimental purposes
*	ERLINK	Execution error diagnostics program

3) Molecular Physics
   Computation of Vibration-Rotation Matrix Elements for
   Diatomic Molecules

   Dr. W. Benesch, Institute for Molecular Physics

   The Institute for Molecular Physics is concerned with a
variety of research projects in the general categories of
physical chemistry, spectroscopy, thermodynamics, statistical
mechanics and kinetic theory, and molecular scattering phe-
nomena.

   The problem with which this investigation is concerned
is that of computing the vibrational matrix elements for
dipole transitions of a rotating diatomic molecule. There is
a considerable background of effort in this area, although
most work has been carried out on total vibration-rotation
bands. The present program seeks to obtain matrix elements
for individual vibration-rotation lines.

   The first computation has generated matrix elements based
on the Morse oscillator wave function and the following dipole
moment function.

$$(1) \quad M = M_o + M_1 (r-r_e) + M_2 (r-r_e)^2 + M_3 (r-r_e)^3.$$

The values obtained have been very helpful in the interpreta-
tion of data resulting from hydrogen iodide intensity mea-
surements. The measured and computed matrix elements are in
good agreement in both the fundamental and overtone bands al-
though the development of certain trends at the highest values
of the rotational quantum number, J, indicated that the centri-
fugal stretching might have been treated more vigorously.

   In an effort to improve the J-dependence of the results,
the next computation carried out was based on perturbed har-
monic oscillator wave functions suggested by Herman and Wallis
and the dipole moment function (1). The core of the computa-
tion was a Simpson's Rule integration of the eight integrals
which are needed for application to the two branches.

   As a result of the inclusion of an addition term in the
expansion of the centrifugal stretching term, the J-dependence
of the results was, indeed, improved, so that these calcula-
tions constitute the best theoretical representations of the
fundamental line intensities of hydrogen iodide and hydrogen
bromide.

Since the potential function upon which the Herman and Wallis wave functions are based is quite unrealistic, the computation which is most successful in the fundamental is not readily extended to the overtone band. Accordingly, it was considered worthwhile at this point to turn to a direct numerical integration of the radial Schroedinger equation appropriate to this problem, and current efforts are being directed toward an application of the Numerov method to obtain the first three eigenfunctions of the problem, after which the computation will revert to the matrix element integration employed in the previous method.

4) Physics and Astronomy

a) Computer Program Development in Long Wavelength Radio Astronomy

Dr. W. C. Erikson, Department of Physics & Astronomy

As radio waves propagate through the solar corona, they undergo scattering due to the fact that the electron density, and thus the index of refraction, varies irregularly from point to point. The observation of these scattering phenomena yield valuable data concerning the structure of the solar corona, and such observations have been pursued actively for nearly a decade. The long wavelength of 11.4 m employed at the antenna of the Clark Lake observatory in California, is very sensitive to coronal scattering and permits the examination of the scattering phenomena with great resolution.

The operation of the Clark Lake observatory has recently been assumed by the Department of Physics and Astronomy of the University of Maryland. W. C. Erickson will direct the research with the antenna.

In order to prepare for the future extensive computational work connected with the reduction and analysis of the radio-astronomical observations, it was necessary to develop a basic set of special and particularly efficient computer programs. During the past four months essentially two such programs have been developed and checked out. The first program takes the raw data as it is produced by the telescope, makes all corrections for beam width, position, precession, and the like, and yields processed data concerning the position, angular size, and intensity of

radio stars. The second program will be used in the reduction of solar data. It solves certain spherical trigonometrical problems which are routine but very repetitious and tedious. For each day it computes the position of the sun in each of the 70 lobes of the antenna's response pattern along with various other parameters such as the great circle distances between the sun and certain radio sources.

The development of these programs represented an important first phase in the computer-oriented part of this research effort. It is expected that future production-type use of these programs will be supported from other sources.

b)   <u>Computational Methods in Nuclear Physics</u>

Dr. J. B. Marion, Dr. A. Jaffe, Dr. R. Detenbeck, Dr. W. Greiner, Department of Physics and Astronomy

The principal instrument of the University of Maryland's experimental nuclear physics program is the 3.5 million-volt Van de Graaff accelerator. The research programs revolve about the study of the interactions of various particles, such as protons, deuterons, and helium ions, with other nuclei, mainly emphasizing reactions with with the light nuclei.

The research projects have been described in detail in our proposal for this grant, NsG 398. In order to stimulate the computer-oriented work in this research area it was necessary to begin with the development of several computer programs for the reduction of experimental results. Essentially three sets of such programs have been completed:

<u>Nuclear Reaction Kinematics</u>: (A. Jaffe) An efficient program has been developed for the study of nuclear reaction kinematics, specifically, (a)as an aid in the identification of reaction products, (b)for the reduction of data to the center-of-mass system. The non-relativistic equations have been used. (See, e.g., J. B. Marion, Nuclear Data Tables, Part III, 1960)

<u>Magnet Calibrations</u>: (J. B. Marion) The Van de Graaff accelerator produces a beam of particles which is analyzed

in momentum by a uniform field magnet. The magnetic field
is measured by a nuclear magnetic resonance device. The
output frequency is then related to the energy of the par-
ticle beam by a certain relativistic formula.

A computer program has been developed which relates
the frequency to the energy of every type of particle that
is being used in the Maryland accelerator.

Transformation Tables: (R. Detenbeck and J. B. Marion)
During nuclear experiments it is frequently necessary to
compute rapidly the energies of particles emerging from
nuclear reactions and to transform experimentally measured
quantities from the laboratory system to the theoretically
significant center-of-mass system. These computations are
usually handled on a computer (see first program), but
in many experiments it is desirable to have a set of tables
available for such kinematics transformations.

A program has been prepared to print such a set of
tables in proper format for direct photographic reproduc-
tions. It is planned to publish these tables -- if possi-
ble -- through the Government Printing Office.

Parallel with the development of these three programs
the following new computational research project was begun:

Three Body Reactions, Phase Space, and Coulomb
Penetrabilities: (R. Detenbeck and U. Gerlach) Improve-
ments in experimental techniques and computational proce-
dures have now made it possible to study three dimensional
reactions of the type

$$N^{14} \; (p, \; 2p) \; C^{13}$$
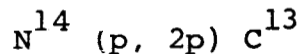
in some detail. It is now possible to measure energy and
angular distributions of both light particles. These will
depend on whether the two light particles emerge simultan-
eously or one-after-another. If both particles emerge
simultaneously and the transition rate for the reaction is
energy insensitive, the energy distributions of the emer-
gent particles are calculable from phase-space considera-
tions. An example of such a calculation is contained in a
report by Berlin and Owen (Johns Hopkins University, 1957).

When the emerging particles are charged, the assumption

of an energy-independent transition rate is not valid.
The particular phase-space calculation of Berlin and Owen
has been modified to include a correction for Coulomb
forces. Although the exact three-body Coulomb-force pro-
blem cannot be solved, the most important effects are in-
cluded by taking into account the interaction between the
pair of particles with lowest ratio of "relative energy"
to "Coulomb energy". The correction would be more accu-
rate if it used exact two-body Coulomb wave functions
(or even better, optical model wave functions). But for
simplicity the program developed uses only the Gamow pene-
tration factors for the appropriate pairs of particles.

Fixing the incident beam energy and the position of
one of two detectors connected to record particle pairs
in time coincidence, the experimenter measures the reac-
tion yield as a function of the position of the second
detector and the energy deposited therein. The program
calculates a predicted yield for such a situation, assum-
ing a one-step reaction, taking Coulomb forces into ac-
count approximately. The program will be most accurate
in two regions:

a) where Coulomb forces are negligible (of course);

b) where the Coulomb penetration factor dominates the
reaction rate; i.e., where the relative energy of
one charged pair (and unfortunately the reaction
yield) is very low.

The program will be least accurate where the relative
energy of one charged pair is near the Coulomb barrier.
This is unfortunate, but should still permit a study of
qualitative Coulomb effects. The equations used are non-
relativistic.

Giant Dipole Resonance - Collective Level Shift Com-
putations: (W. Greiner) The shell-model theory of the
giant dipole resonance is based upon starting with accurate
single-nucleon wave functions as solutions of the Hartree-
Fock self-consistent field. When only bound state wave
functions are involved, reasonable accuracy can be obtained
by the harmonic oscillator approximation. This is, how-
ever, no longer true in the more realistic situation where
the important excitations are free, or unbound states of
the nucleus. In this case the single-nucleon wave functions

are in reality scattering states and lend themselves to
no simple analytic approximation. It is necessary to
evaluate them numerically on a computer.

This project is presently concerned with investigating the shift of the collective giant-resonance levels
in O^{16} due to the interaction of these bound levels with
continuum states. This interaction takes place via residual forces, which have not been included in the shell-
model field.

Up to now we have calculated the shift due to virtual neutron emission and we have found that it is of the
order of 0.6 MeV, a quite appreciable correction to the
usual particle-hole calculations.

The work is now continuing with the computation of the
same effect for virtual proton emission. For this purpose it is necessary to develop special programs for the
evaluation of regular and irregular Coulomb wave functions.

5. Chemical Engineering

During the report period we have begun to help the Department of Chemical Engineering with the computer-oriented phases
of several research projects. Analysis - and programming -
problems have so far limited the extent of this computational
research, but we expect that this situation will improve in
the next few months.

a) Investigation of Complex Equilibrium Stage Processes

Dr. J. Marchello, Department of Chemical Engineering

Together with several of his graduate students,
J. Marchello began an investigation on complex equili-
brium stage processes. This project deals with design
computations for distillation, absorption, extraction and
several other processes that are conducted in cascades in
a stage-wise fashion. This computational work involves
the sequential stage-by-stage material - and energy -
calculations for such processes, with the emphasis being
on multicomponent systems. A new approach to the problem
of computing the required number of stages has been de-
vised, but this method is still encountering certain con-
vergence problems and is therefore not yet completely

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satisfactory. New methods of attack are now being studied.

b) Computer Modeling of Two-phase Flow Problems

Dr. A. Gomezplata and C. Nichols, Department of
Chemical Engineering

A. Gomezplata together with C. Nichols, a doctoral
candidate, is studying a problem of two-phase flow. Air
and water are mixed and forced through a vertical test
section where voids and pressure losses are measured. A
computational procedure based on theoretical two-phase
models is employed to correlate void fraction data. So
far, the results obtained show that models taking into
account velocity and void fraction distribution can be
used effectively to predict downflow data. On the other
hand, it was also shown that lumped-parameter models can-
not differentiate between upflow and downflow systems.

IV. Computer Use Supported by the Grant

The following table gives a detailed breakdown of the computer time supported by the NASA Grant NsG 398 for the time period March through August 1963. The breakdown is given by areas of interest instead of by specific projects. A more detailed breakdown is available upon request.

Table of Computer Time
Supported by NASA Grant NsG 398

(All times are given in hours, minutes and seconds.)

	March	April	May	June	July	August	Total
Programming Systems	11-45-27	10-20-40	4-48-38	15-46-38	6-23-37	12-05-08	61-10-08
Numerical Mathematics	0-33-58	16-26-29	28-29-48	11-04-28	8-59-50	3-53-39	69-28-12
Crystallography	4-34-59	36-13-42	22-27-39	6-27-06	0-0-0	0-0-0	69-43-26
Molecular Physics	-	-	-	0-20-32	0-37-59	0-23-51	1-22-22
Physics & Astronomy	0-45-00	0-12-31	2-40-32	5-58-25	0-40-38	4-14-05	14-31-11
Chemical Engineering	-	-	2-20-37	0-0-0	0-0-0	0-0-0	2-20-37
Totals	17-39-24	63-13-22	60-47-14	39-37-09	16-42-04	20-36-43	218-35-56